

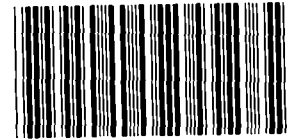
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Multiphase Equation of State for Iron

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Multiphase Equation of State for Iron

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Abstract

The PANDA code is used to build a multiphase equation of state (EOS) table for iron. Separate EOS tables were first constructed for each of the individual phases. The phase diagram and multiphase EOS were then determined from the Helmholtz free energies. The model includes four solid phases (α , γ , δ , and ϵ) and a fluid phase (including the liquid, vapor, and supercritical regions). The model gives good agreement with experimental thermophysical data, static compression data, phase boundaries, and shock-wave measurements. Contributions from thermal electronic excitation, computed from a quantum-statistical-mechanical model, were found to be very important. This EOS covers a wide range of densities (0 - 1000 g/cm³) and temperatures (0 - 1.2×10⁷K). It is also applicable to RHA steel. The new EOS is used in hydrocode simulations of plate impact experiments, a nylon ball impact on steel, and the shaped charge perforation of an RHA plate. The new EOS table can be accessed through the SNL-SESAME library as material number 2150.

Acknowledgment

An improved equation of state (EOS) for iron, one that includes a realistic treatment of its interesting phase diagram, is long overdue. This work was undertaken after a survey of various CTH users indicated that the highest priority for new EOS should be assigned to iron and RHA steel. I am grateful to Gene Hertel for conducting this survey, to those who participated in it, and to DARPA for funding. I also thank Paul Yarrington for his support and encouragement, and Charlie Anderson, for sending me the shock data for RHA.

As always, I thank my wife Donna, whose love, prayers, and encouragement are what keep me going.

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Tables

Table 1. EOS Constants for Solid Models

Symbols and Units

ρ	density [g/cm^3]
V	specific volume, $V = 1/\rho$ [cm^3/g]
T	temperature [K]
P	pressure [GPa]
E	specific internal energy [MJ/kg]
A	Helmholtz free energy [MJ/kg]
S	entropy [$MJ/(kg \cdot K)$]
C_V	constant volume specific heat, $C_V = (\partial E / \partial T)_V$ [$MJ/(kg \cdot K)$]
β	isothermal bulk modulus, $\beta = \rho (\partial P / \partial \rho)_T$ [GPa]
Γ	Grüneisen function [unitless]
Θ	Debye temperature [K]
$\phi(\mathbf{x}_s)$	atomic potential function (\mathbf{x}_s are coordinates of neighbors)
c_s	sound velocity [km/s]
u_s	shock velocity [km/s]
u_p	particle velocity [km/s]

1. Introduction

The equation of state (EOS) of iron has long been a topic of considerable interest, and there is now a vast literature devoted to it [1] - [5]. This fact is hardly surprising, in view of the importance of iron and its alloys as structural materials. However, much work has also been motivated by interest in modeling the earth's core [4], a problem requiring an understanding of the properties of iron at high temperatures and pressures (3000-7000K, 200-400 GPa). The present work was undertaken to provide an improved EOS for use in armor penetration studies and other impact problems at low, intermediate, and high velocities. Finally, the complexities of the phase diagram and other intriguing properties of iron make it a leading candidate for basic research studies.

Four solid phases of iron have been observed [6]. The alpha phase, which is stable at ambient pressure and temperature, has a bcc structure and exhibits well-known magnetic properties up to the Curie temperature of 1042K [7]. Iron transforms to the gamma phase, which has an fcc structure, at temperatures above 1184K (and zero pressure) [7]. It transforms back to the bcc structure (sometimes called the delta phase) at 1665K before melting at 1809K [7]. The epsilon phase, which was first discovered in shock wave experiments [2], has an hcp structure and is produced at pressures above about 11 GPa [5]. The boiling point of iron is 3135K [7]. The properties and boundaries of the various phases as functions of pressure and temperature have been studied experimentally, using both static and dynamic methods.

In this work, we have used the Panda code [8], which provides the tools needed to model materials having complicated phase diagrams. For example, we have successfully used this method to model the properties of calcium carbonate minerals [9]. Our application of the technique to iron can be summarized as follows:

- Individual tables of thermodynamic properties were constructed for the α , γ , and ϵ phases by combining contributions from the 0K isotherm, lattice vibrations, and thermal electronic excitations. In addition, a magnetic contribution was included for the α -phase.
- A table of the thermodynamic properties for the fluid phase was constructed using fluid perturbation theory [10] to treat the atomic motions, together with the thermal electronic term. The fluid EOS describes not only the liquid, but also the vapor and supercritical regimes.
- Experimental data were used to determine the model parameters wherever possible. The thermal electronic term, which was calculated from an *a priori* model, was found to have a surprisingly large effect upon the thermal expansion of iron as well as its heat capacity.
- A multiphase EOS table was constructed from the EOS tables for the individual phases, assuming thermodynamic equilibrium. Hence, the phase boundaries

were determined by finding the phase having the lowest Gibbs free energy at a given pressure and temperature.

- The multiphase EOS can be used by hydrodynamics codes that have the capability to read the SESAME tabular format, as described in Refs. [11] and [12]. In this way, one can make use of detailed and sophisticated features that could not be included in any analytic EOS model.

The theoretical model is described in Sec. 2 and Appendix A. The Panda output file generated during the multiphase EOS calculation is given in Appendix B. In Sec. 3, we discuss the results of the model and compare them with experimental measurements of thermophysical properties, static compression curves, the phase diagram, and shock wave behavior. In Sec. 4, we discuss hydrocode calculations, made using the CTH code and our new EOS table, of plate impact tests, of the impact of a nylon ball on a steel plate, and of the shaped charge perforation of an RHA plate.

2. Description of the Model

2.1 Solid Phases

The thermodynamic functions for the α , γ , and ϵ phases are assumed to have the following form:

$$P(\rho, T) = P_c(\rho) + P_l(\rho, T) + P_m(\rho, T) + P_e(\rho, T), \quad (1)$$

$$E(\rho, T) = E_c(\rho) + E_l(\rho, T) + E_m(\rho, T) + E_e(\rho, T) - \Delta E_b, \quad (2)$$

and

$$A(\rho, T) = E_c(\rho) + A_l(\rho, T) + A_m(\rho, T) + A_e(\rho, T) - \Delta E_b. \quad (3)$$

Here the subscripts c , l , m , and e denote contributions from the zero-Kelvin curve, lattice vibrations (including the zero-point term), magnetic excitations (α -phase only), and thermal electronic excitations, respectively. ΔE_b is the cohesive energy, which is subtracted in order to give a consistent energy zero for all three phases; values for this constant [13], corrected for the zero-point lattice energy [8], are given in Table 1.

Modern static pressure devices have been used to measure the compression curves for the α and ϵ phases at room temperature [14] - [18] and also at temperatures up to 723K [17]. These various sets of data were corrected to 0K, by subtracting off the calculated thermal pressure corrections P_l and P_e , and fit to the Birch-Murnaghan equation [19],

$$P_c(\rho) = \frac{3}{2}\beta_0(\eta^{7/3} - \eta^{5/3}) \left[1 + \frac{3}{4}(\eta^{2/3} - 1)(\beta'_0 - 4) \right], \quad (4)$$

where $\eta = \rho/\rho_0$, and ρ_0 , β_0 , and β'_0 are constants, given in Table 1. For the γ -phase, the value of ρ_0 was fixed by fitting the thermal expansion data, and β_0 and β'_0 were taken to be intermediate between values for the α and ϵ phases. The γ -phase parameters are also constrained somewhat by the shock data for porous iron. The zero-Kelvin curves were input to Panda using the tabular cold curve option [8], which computes a thermodynamically consistent energy E_c . To insure correct asymptotic behavior at high densities, an extrapolation formula based on Thomas-Fermi theory [8] was used for $\rho > 11.0 \text{ g/cm}^3$ (i.e. $P_c > 100 \text{ GPa}$).

The contributions from lattice vibrations were calculated using the Debye model with a cutoff in the sum over the levels, as implemented in Panda [8]. Input to this model includes the Debye temperature Θ_{ref} and Grüneisen parameter Γ_{ref} at the room temperature solid density ρ_{ref} , and a constant τ , which specifies the density dependence of the Grüneisen function,

$$\Gamma(\rho) = (\Gamma_{ref} - 0.5) (\rho_{ref}/\rho)^\tau - 0.5. \quad (5)$$

Values of Θ_{ref} for the α and γ phases were determined by fitting the model to heat capacity data [7]. Θ_{ref} for the ϵ -phase was taken from Stepakoff and Kaufman [20], who estimated it from the heat capacity of ϵ -stabilized Ru alloys. Values of Γ_{ref} for the α and γ phases were determined from thermal expansion data [6] [21]. Γ_{ref} for the ϵ -phase was chosen by fitting the model to the high temperature PVT data of Huang, et. al. [17]. The “typical” value $\tau = 1$ was used for the α and γ phases, but it was found that better results for the γ - ϵ phase boundary were obtained by making Γ for the ϵ -phase fall off more rapidly with density. Since the ϵ -phase has such a high value for Γ_{ref} , $\tau = 2$ also gives a value of Γ comparable to that for the other two phases at high densities.

TABLE 1: EOS Constants for Solid Models

parameter	α -phase	γ -phase	ϵ -phase
ΔE_b	7.397	7.337	7.397
$\rho_0, \text{g/cm}^3$	7.969	8.060	8.430
β_0, GPa	173.0	174.0	182.0
β'_0	4.80	4.70	5.00
Θ_{ref}, K	425.0	300.0	385.0
Γ_{ref}	1.70	1.65	2.40
ρ_{ref}	7.873	7.953	8.264
τ	1.0	1.0	2.0
$k, \text{MJ/kg/K}^{2.5}$	1.36×10^{-6}	-	-
T_0, K	1080.0	-	-

The magnetic term, included only for the α -phase, was treated in a manner similar to that used by Andrews [1]. He noted that, since the Curie temperature is nearly independent of pressure, it is a good approximation to take the magnetic term as independent of density. As a result, the magnetic term makes no contribution to the pressure ($P_m = 0$). He used the following empirical formula to represent the magnetic contribution to the heat capacity below the Curie temperature:

$$C_{Vm}(T) = kT^{1.5}/(T_0 - T), \quad (6)$$

where the constants k and T_0 , together with other model parameters, were adjusted to match experimental data. Our values for these constants differ from those used by Andrews, because our model for the thermal electronic term predicts larger contributions than his. For the same reason, we simply set $C_{Vm} = 0$ above the Curie point, where Andrews used an expression that approaches zero at high temperatures. Equation (6) was integrated numerically to obtain the energy and free energy and input to Panda using the tabular option [8].

The thermal electronic term is discussed in Sec. 2.3.

2.2 Fluid Phases

The thermodynamic functions for the fluid phases (liquid, vapor, and supercritical fluid) are computed using a version of liquid perturbation theory called the CRIS model [10]. Since this model has been discussed in detail in previous work, we will discuss only a few points here. The Helmholtz free energy is given by

$$A(\rho, T) = A_\phi(\rho, T) + A_e(\rho, T) - \Delta E_b. \quad (7)$$

Here A_ϕ includes both the contributions from electronic binding, in the ground state configuration, and the thermal atomic motion in the force field created by the electrons. (It corresponds to $E_c + A_l$ in Eq. (3), but these two terms are not additive as they are in the solid model.) A_e is the contribution from thermal electronic excitations; the same model is used for the solid and fluid phases and is discussed in Sec. 2.3. ΔE_b is the cohesive energy, which is subtracted to give the same energy zero as for the solid phases. The other thermodynamic quantities are computed from standard thermodynamic relations [8] [10].

In order to compute the properties of a fluid, it is necessary to know something about the function ϕ , which we define as the potential energy of an atom in the field of neighboring atoms. This function, which is determined by the intermolecular forces, is related to the energy of the solid on the zero-Kelvin isotherm by

$$E_c(\rho) = (N_0/W) \phi(\mathbf{x}_s), \quad (8)$$

where N_0 is Avogadro's number, W is the atomic weight, and \mathbf{x}_s denotes the configuration of the neighbors in the solid at density ρ . For the calculation of fluid properties, ϕ must be averaged over many configurations of neighbors that are different from those of the solid. Since current theories of the electronic structure of matter are not sufficiently accurate for calculating ϕ , except for very simple systems, the CRIS model idealizes the fluid configurations and approximates ϕ by [10]

$$\phi \approx (\rho/\rho_s) E_c(\rho_s). \quad (9)$$

Here ρ is the actual density of the fluid, and ρ_s is the solid density having the same nearest neighbor distance as that of the given fluid configuration.

For materials like iron, with more than one solid phase, there is ambiguity as to which zero-Kelvin isotherm E_c to use in Eq. (9). However, our experience has shown that E_c for the most dense solid phase tends to give the best predictions of the fluid properties. In this work, therefore, we use the same function E_c for the fluid as for the hcp (ϵ) phase. As a result, the cohesive energy ΔE_b is also the same for both phases.

It is well-known that perturbation theory can be used to expand the free energy A_ϕ about the properties of a hard-sphere fluid [10],

$$A_\phi(\rho, T) = A_0(\rho, T, \sigma) + (N/W) \langle \phi \rangle_0 + \Delta A. \quad (10)$$

Here A_0 is the free energy for a fluid of hard spheres with diameter σ , and $\langle \phi \rangle_0$, the first-order correction, is an average of ϕ over all configurations of the hard sphere fluid. By definition, ΔA includes all corrections to the first two terms.

In the CRIS model, the hard-sphere diameter σ is defined by a variational principle that minimizes $|\Delta A|$. The correction terms are then computed from approximate expressions. The variational principle insures that the structure of the hard-sphere system used in the perturbation expansion is close to that of the real fluid. We have previously demonstrated that this approach does in fact give good results for the structure factor of iron, and also its shear viscosity [3] [10].

The following additional steps were taken to “fine tune” the fluid model to give the best possible agreement with experimental data for liquid iron. First, the Panda LJ MATCH option, which defines the behavior of the zero-Kelvin isotherm in tension [8], was used to adjust the liquid density at the melting point [22]. Second, the parameter EFAC, an empirical correction to Eq. (9) [8], was used to adjust the energy at the melting point [7]. Finally, we modified Panda so that the two integrals computed in the correction term ΔA could be multiplied by empirical factors, WX1 and WX2; these factors were used to adjust both the energy and the entropy at the melting point [7]. The values used were RLJ=7.5, FAC LJ=0.68, EFAC=0.23, WX1=WX2=2.1.

2.3 Thermal Electronic Contributions

At sufficiently high temperatures, excitation of electrons out of the ground state configuration can make an important contribution to the thermodynamic properties [23]. Most EOS models for iron have either ignored this term or attempted to represent it using simple free electron gas formulas. The model used here predicts that the thermal electronic term becomes important at temperatures above about 500K and that it makes a large contribution to the thermal expansion. The latter effect, which agrees with experimental data, is not predicted by the simpler models.

None of the existing theories for calculating thermal electronic contributions to the EOS give satisfactory results over the full density-temperature range of interest [23]. Therefore, we have synthesized this term by combining results from two theories - the INFERNO model of Liberman [24] for densities $\rho > 6 \text{ g/cm}^3$, and the Panda ionization equilibrium (IONEQ) model [8] for densities $\rho < 1 \text{ g/cm}^3$, with an average of the two models at intermediate densities. These data were combined to form a table of the electronic entropy, the features of which are depicted in Fig. 1. The other thermodynamic functions were computed by numerical differentiation and integration of the entropy, as described in Ref. [8]. The electronic pressure is shown in Fig. 2.

An important aspect of the electronic behavior of matter is the *insulator-metal transition* - the change of the valence electrons from localized, insulating states at low densities to delocalized, metallic states at high densities. Previous work showed that the INFERNO

model gives excellent predictions of the effect of this phenomenon on the shock Hugoniot of xenon, in which the transition is induced under pressure [3] [10]. In iron, the insulator-metal transition begins at a density of about 4 g/cm^3 , causing a pronounced drop-off in the entropy. At densities above about 20 g/cm^3 , the electrons behave like a simple free electron gas. The same phenomenon causes large thermal electronic contributions to the pressure in the density range $4 < \rho < 20$, as seen in Fig. 2.

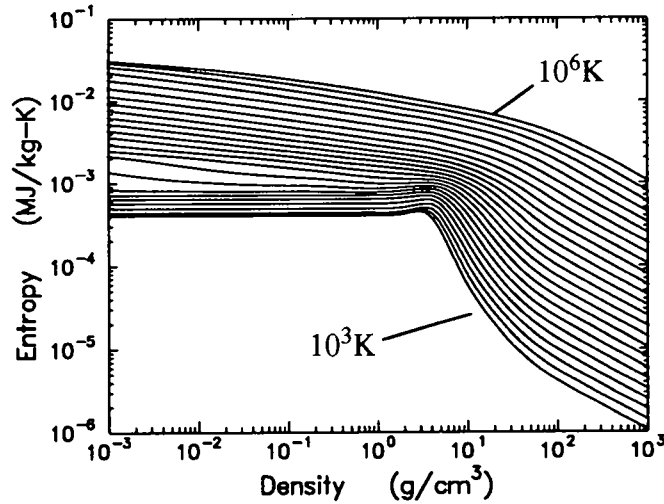


Fig. 1. Electronic contribution to the entropy for iron. Temperatures on the 25 isotherms shown range from 1.0×10^3 to $1.0 \times 10^6 \text{ K}$ and are equally spaced in the logarithm.

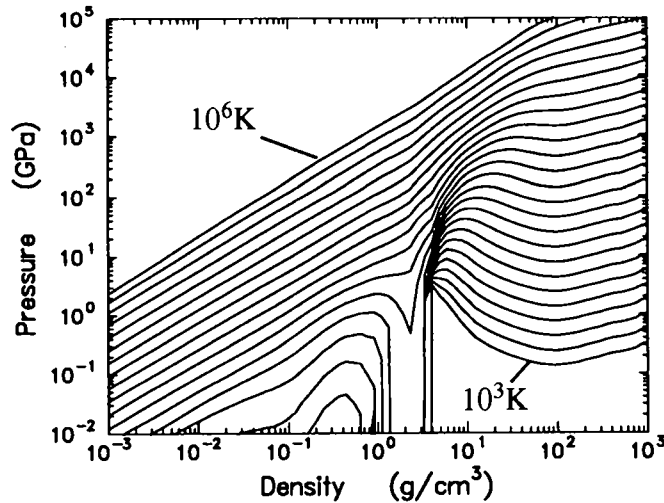


Fig. 2. Electronic contribution to the pressure for iron. Isotherms are the same as Fig. 1.

The INFERNO and IONEQ models both exhibit the basic features seen in Figs. 1 and 2. However, the INFERNO model is preferred in the high density regime because it has a more sophisticated and self-consistent treatment of the continuum lowering and metalliza-

tion effects. It predicts the low-temperature coefficient of the electronic specific heat to be 1.4×10^{-3} cal/mole/K², in excellent agreement with the value reported for the ϵ -phase [20], and only slightly higher than the value of 1.2×10^{-3} reported for the α -phase [7]. (The value for the α -phase may include magnetic effects that are ignored here.) The INFERNO calculations are also in good agreement with band theoretical calculations of Boness and Brown [25], which encompass densities and temperatures up to 14 g/cm³ and 1.0×10^4 K, respectively.

The switch to a different model at low densities is necessary because INFERNO uses an approximation for the statistics of the bound state configurations that is very inaccurate in the insulating regime. The calculations also become prohibitively expensive, due to the existence of many bound states. The IONEQ results are in fairly good agreement with those from INFERNO in the regime $\rho > 4$. However, some modifications to them were needed in order to make an entropy table that was smooth enough for computing the pressure by numerical differentiation. Additional details about construction of the electronic entropy table are given in Appendix A.

2.4 Multiphase EOS Calculations

After tabulating EOS for the α , γ , ϵ , and fluid phases, the Panda MOD TRN option [8] was used to compute the phase diagram and construct the multiphase EOS. The input for this option includes an energy shift for each phase, which was chosen to give zero energy for the α -phase at room temperature and solid density. In principle, the same energy shift should be used for all four phases, since all four tables have the same zero of energy. However, slightly different values were used in order to refine the predicted phase boundaries.

We were unable to find a satisfactory model for the α -phase that described both the low-temperature ($T < 1184$ K) and high-temperature (δ -phase) regions. Therefore, a second table was made for the δ -phase. By adding a constant to the entropy ($WSL = 1.42$ [8]), and using a different energy shift than for the low-temperature region, it was possible to match the γ - δ transition temperature, melting temperature, and slope of the melting curve.

The energy shift for the ϵ -phase was chosen to make the α - ϵ phase boundary occur at 13.0 GPa, consistent with shock loading data, instead of the equilibrium value, 11.0 GPa.

The mesh used in making the multi-phase EOS table included 90 densities in the range $1.0 \times 10^{-6} \leq \rho \leq 1.0 \times 10^3$, plus a $\rho = 0$ point, and 70 temperatures in the range $0 \leq T \leq 1.2 \times 10^7$. The mesh points were chosen to give good resolution of the phase transitions and other important features of the EOS surface. In order to allow treatment of fracture models, a tension region was included at temperatures below the boiling point ($TSPALL = 3135$). In order to model the vaporization behavior, Maxwell constructions were performed at all higher temperatures, up to the critical point ($\approx 2.5 \times 10^4$ K).

The new EOS table has been added to the SNL-SESAME library [11] (file “sesame”) as material number 2150.

3. Results and Discussion

3.1 Thermophysical Data

Calculated curves of entropy and density, as functions of temperature, are shown in Figs. 3 and 4, respectively, along with experimental data [7] [21] [22]. To illustrate the importance of the thermal electronic contribution, we also show results obtained when this term is omitted. The electronic term makes a significant contribution to both the entropy and the density. It becomes important above about 500K and is quite large in the liquid phase.

The effect on density may explain anomalous behavior that is seen in the thermal expansion data of iron. Andrews pointed out that there is a hump in the thermal expansivity curve, in the range 400-900K, which cannot be fit using a standard treatment of the lattice vibrations and does not correlate with magnetic effects [1]. This behavior was tentatively ascribed to the presence of impurities [20]. However, the present work suggests that it is due to the large electronic pressure term shown in Fig. 2.

The general agreement with experimental data is quite good, although there is some deviation from the measured liquid entropy and density at high temperatures. (The entropy data at high temperatures are actually extrapolations that assume a constant heat capacity for the liquid [7].) Our theory of the thermal electronic contributions is admittedly weakest in the density range $1 < \rho < 6$, where the two models are being joined. Hence it is likely that most of the discrepancy arises from the treatment of that term.

Our calculated boiling point for iron is 3190K, quite close to the experimental value of 3135K [7]. The critical temperature, which is strongly influenced by the thermal electronic term, is predicted to be $\approx 2.5 \times 10^4$ K. There are no measurements of the critical point or the vaporization behavior at high temperatures.

3.2 Static Compression Data

In Fig. 5, we compare the room temperature isotherm computed using our model with the experimental data [14] - [18]. The insert in Fig. 5 shows data to a pressure of 300 GPa. The agreement is excellent up to 100 GPa, but our model is slightly softer than recent measurements relative to a Pt standard [18] at higher pressures. (We have used the extrapolation formula in this regime.) We have not been able to bring our curve into agreement with these data without spoiling our predictions of the shock data. Therefore, we have decided to accept this discrepancy, at least for the present.

As noted in Sec. 2.1, the model parameters were chosen to give good agreement with static measurements for α - and ϵ -phase iron at temperatures up to 723K [17], although we have not displayed those data here.

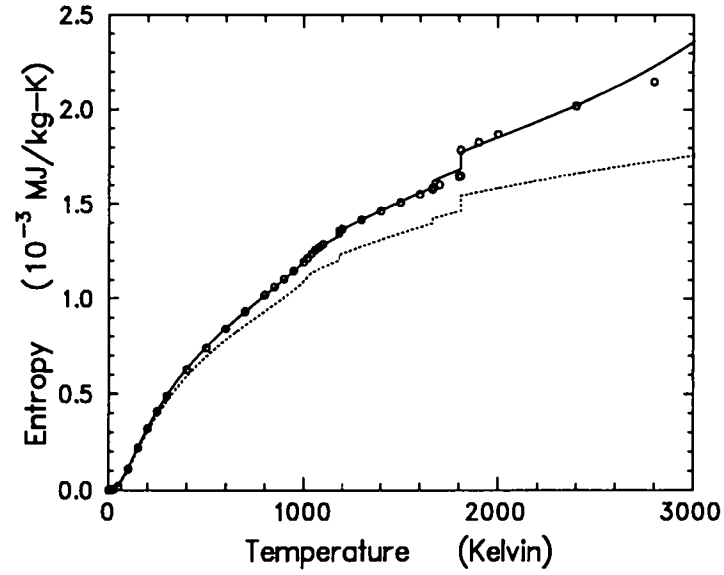


Fig. 3. Entropy vs. temperature for iron (zero pressure). The solid line is calculated including all terms, the dotted line omitting the thermal electronic term. Circles are experimental data [7].

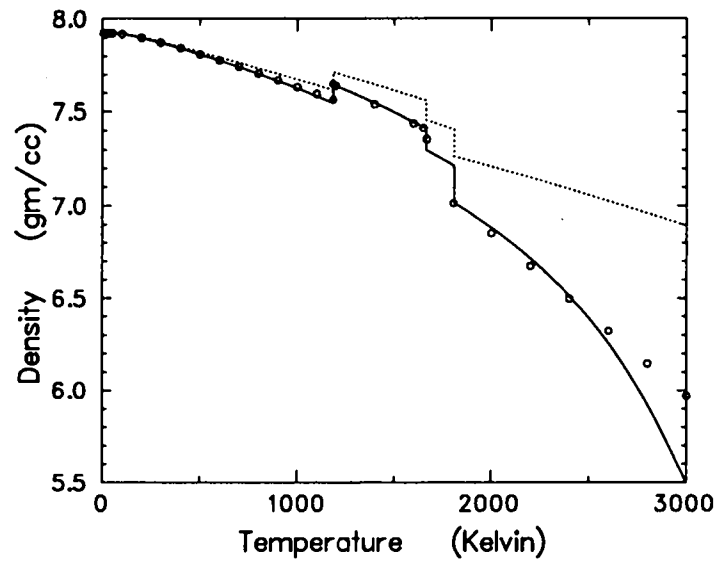


Fig. 4. Density vs. temperature for iron (zero pressure). The solid line is calculated including all terms, the dotted line omitting the thermal electronic term. Circles are experimental data [21] [22].

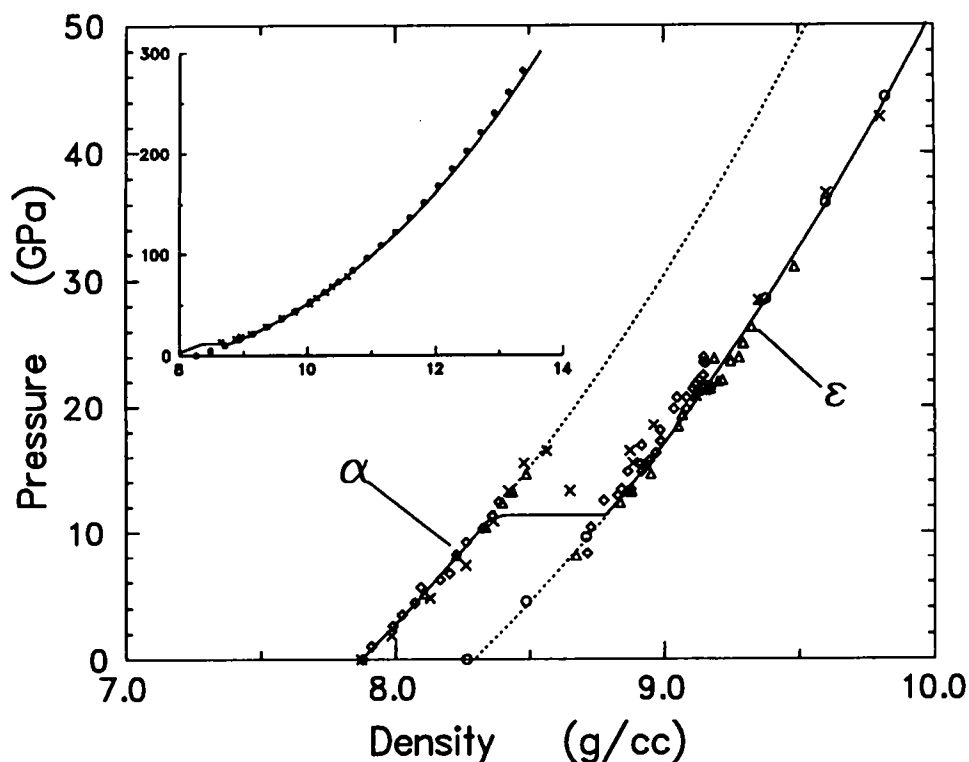


Fig. 5. Comparison of calculated room temperature isotherm (solid line) with diamond cell measurements: triangles - [14], x's - [16], diamonds - [17], circles - [18]. Dotted lines are extrapolations of the α and ϵ curves into their metastable regions. The insert shows data to higher pressures.

3.3 Phase Diagram

The calculated phase diagram is compared with experimental data [5] [26] [27] [28] [29] [30] in Fig. 6. (There is still considerable disagreement among various measurements of the α - ϵ phase boundary [5]; the points shown in Fig. 6 are merely representative.) Our results for the α - γ , α - ϵ , γ - ϵ , γ - δ , and δ -liquid phase boundaries are satisfactory.

The α - ϵ transition exhibits nonequilibrium and hysteretic behavior in both static [5] and dynamic [2] experiments. The transition typically occurs at about 13 GPa on loading and 9 GPa on unloading. That kind of behavior cannot be built into a single EOS table. In the present work, the energy of the ϵ -phase was shifted to match the 13 GPa transition when making the tabular EOS; the dotted curves in Fig. 6 show the phase boundaries corresponding to this case. This choice gives a good prediction of the multiple wave structure that is observed on shock loading, but does not accurately represent unloading behavior.

The CTH EOS package offers provisions for treating nonequilibrium and hysteretic effects using the "two-state" model [11] [12]. The α -phase could be omitted when making the EOS table and treated as the initial state, the progress of the transition being controlled by internal state variables. However, that approach has not been investigated in this work.

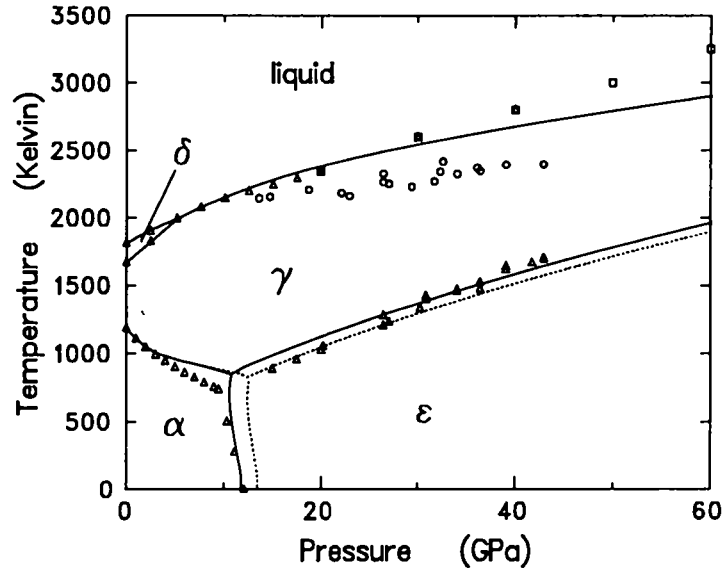


Fig. 6. Phase diagram for iron. Solid line shows equilibrium phase boundaries calculated using the model, and dotted lines show boundaries obtained when the ϵ -phase energy is shifted to give an α - ϵ transition pressure of 13.0 GPa. Experimental data are: triangles - [5] [26] [27] [28], circles - [29], squares - [30].

3.4 Melting

The melting curve and γ - ϵ phase boundary at high pressures are of considerable interest [4] but are not yet well known, experimentally. Our calculated melting curve agrees with the measurements of Strong, et al. [26] and Liu and Bassett [27] up to 20 GPa. At higher pressures, however, there is stark disagreement between the melting data of Boehler [29] and those of Williams, et al. [30]. Our calculated melting curve is intermediate between these two sets of data. However, additional insight into the behavior of these phase transitions at high pressures can be obtained from shock data [31], as discussed below.

3.5 Shock-Wave Behavior

Figure 7 shows the phase diagram and pressure-temperature Hugoniot loci for iron shocked from initial densities in the range 3.4 to 7.85 g/cm³. It can be seen that shock wave measurements for these initial densities sample the phase diagram over a wide range of temperatures and pressures. The calculated Hugoniots agree very well with experimental data [32] - [38] in the shock velocity-particle velocity plane, as shown in Fig. 8.

Brown and McQueen [31] have measured rarefaction wave velocities for iron, shock compressed to pressures between 77 and 400 GPa. They detected two discontinuities that they interpret as due to the ϵ - γ transition (200 ± 2 GPa,) and melting (243 ± 2 GPa). Our model correlates quite well with those results, shown by arrows in Fig. 7.

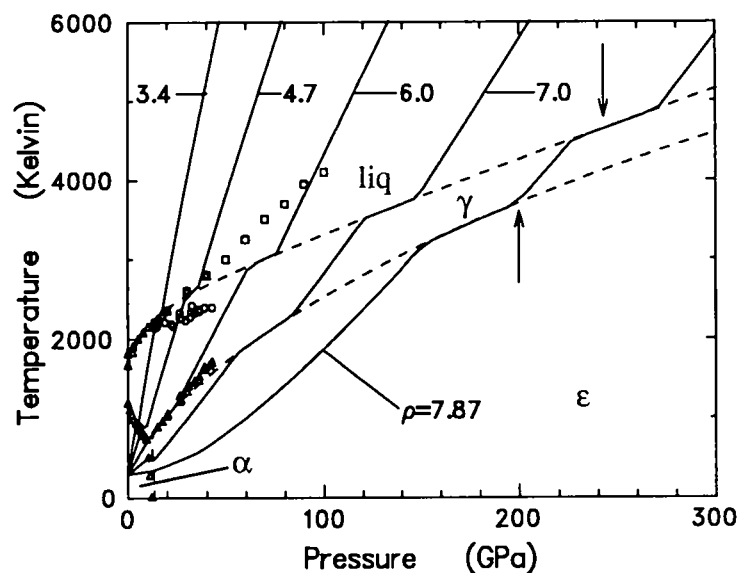


Fig. 7. Shock-induced phase transitions in iron. Solid lines are Hugoniot curves for various initial densities, as indicated, and dotted lines are calculated phase boundaries. Arrows show the pressures at which discontinuities in rarefaction wave velocity are observed in shock wave experiments [31]. Experimental data are the same as in Fig. 6.

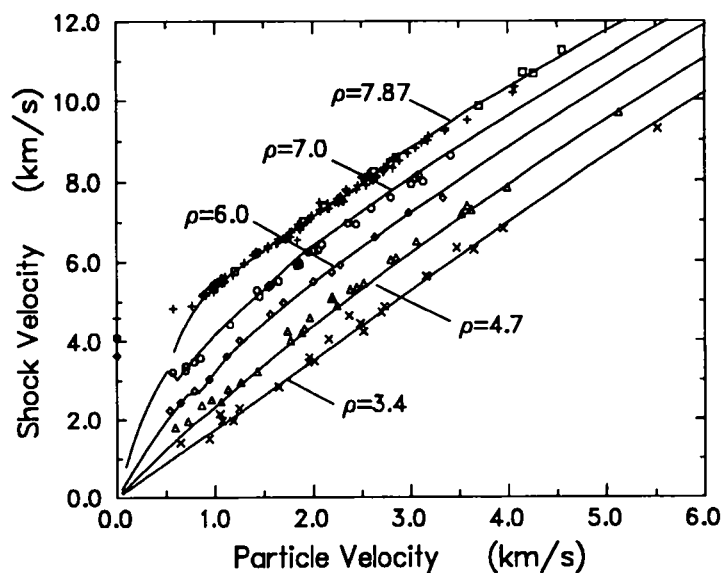


Fig. 8. Hugoniot for iron at various initial densities. Solid lines are calculated. Experimental data are from Refs. [32] - [38].

It should be noted that our model predicts a much lower temperature for shock melting than would be expected from the data of Williams, et. al. [30]. These authors observed that the point obtained by extending the ϵ -phase Hugoniot locus to 243 GPa agrees with an extrapolation of their data. However, that argument fails to account for the lower temperatures obtained after transition to the γ -phase. Our calculations also do not agree with the shock temperatures reported in this paper, but the accuracy of those measurements remains open to question [25]. Drastic changes in our model, which are not warranted by any other data, would be required to reconcile the melting curve of Ref. [30] with the sound speed measurements of Ref. [31]. Therefore, we believe that additional experimental studies of melting in iron are needed.

We further observe that our model predicts that the temperature on the ϵ - γ phase line reaches a maximum at a pressure of about 1×10^4 GPa and that there is no ϵ - γ -liquid triple point, in contrast to other theoretical treatments [4]. It may be possible to modify the parameters for the ϵ and γ phases to introduce a triple point near 300 GPa, without destroying the agreement with the shock melting pressure. However, we have not attempted to do so, since the existing experimental data do not require it.

3.6 RHA Steel

RHA (Rolled Homogeneous Armor) is a mild Ni-Cr steel that has a density and shock wave properties close to those of pure iron. RHA Hugoniot data, for both the α -phase [39] and ϵ -phase [40], are shown in Fig. 9, together with the data for iron [32] [41]. The solid lines show our calculations for an (ideal) initial density of 7.872 g/cm^3 and including the effects of material strength. (The elastic-perfectly plastic model was used with a yield strength and shear modulus of 0.7 GPa and 88.0 GPa, respectively.) The calculations for the α -phase show the elastic precursor with a velocity of 6.0 km/s and the plastic wave for $u_p < 0.32 \text{ km/s}$. For $0.32 < u_p < 0.89$, the calculations account for preshocking of the ϵ -phase by the plastic wave due to the phase transition. (The stress of the first plastic wave was found to be 13.4 GPa when strength was included.) The region $u_p > 0.89$ corresponds to a single plastic wave in the ϵ -phase. (Also see Sec. 4.1.)

Figure 9 shows that the α -phase Hugoniots for RHA [39] and iron [40] are virtually identical within experimental error. Both sets of data lie slightly below our calculations. However, this small discrepancy is eliminated if porosity is taken into account. The dotted line in Fig. 9 shows a calculation for an initial density of 7.84 g/cm^3 , which is typical of actual material samples. The ϵ -phase data for iron and RHA are also in close agreement.

Allowing for experimental uncertainties, there do not appear to be any significant differences between the EOS of iron and that of RHA (although their yield strengths differ). Therefore, we have not constructed a separate EOS table for RHA.

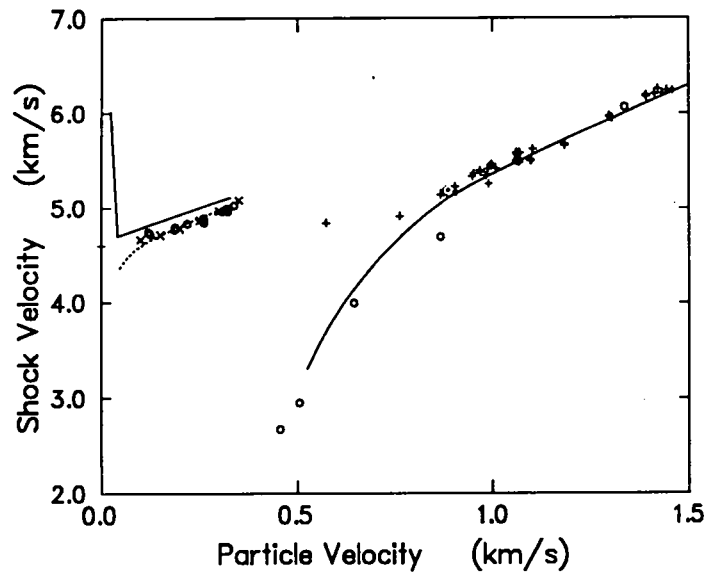


Fig. 9. Hugoniot data for iron and RHA steel. Solid lines are calculated for an initial density of 7.872 g/cm^3 , the dotted line for 7.84 g/cm^3 . Experimental data are: crosses - iron [32], x's - α -phase iron [41], circles - RHA [39] [40].

4. Hydrocode Calculations

4.1 Wave-Profile Measurements

Barker and Hollenbach [42] studied the impacts of iron plates on iron targets at velocities ranging from 0.61 to 1.9 km/s (loading stresses from 12 to 40 GPa). Figure 10 compares CTH calculations, made with our new tabular EOS, with the measured free surface velocities for six of these experiments. The nominal thickness of both the impactor and the target was 0.64 cm in each of these tests. The CTH calculations used a zone size of 0.0032 cm, the elastic-perfectly plastic model with a yield strength and Poisson's ratio of 0.7 GPa and 0.285, respectively, and a fracture strength of 3.8 GPa.

The calculations are in good agreement with the experimental VISAR data. The first wave in all cases is the elastic precursor. Tests 1, 2, 18, and 17 show two plastic waves, the first one being due to the 13 GPa phase transition, and the second being subsequent loading of the ϵ -phase. The phase transition is just at the point of being overdriven in test 6, and is completely overdriven in test 10. Note that the elastic precursor is determined by the properties of the α -phase, even in test 10.

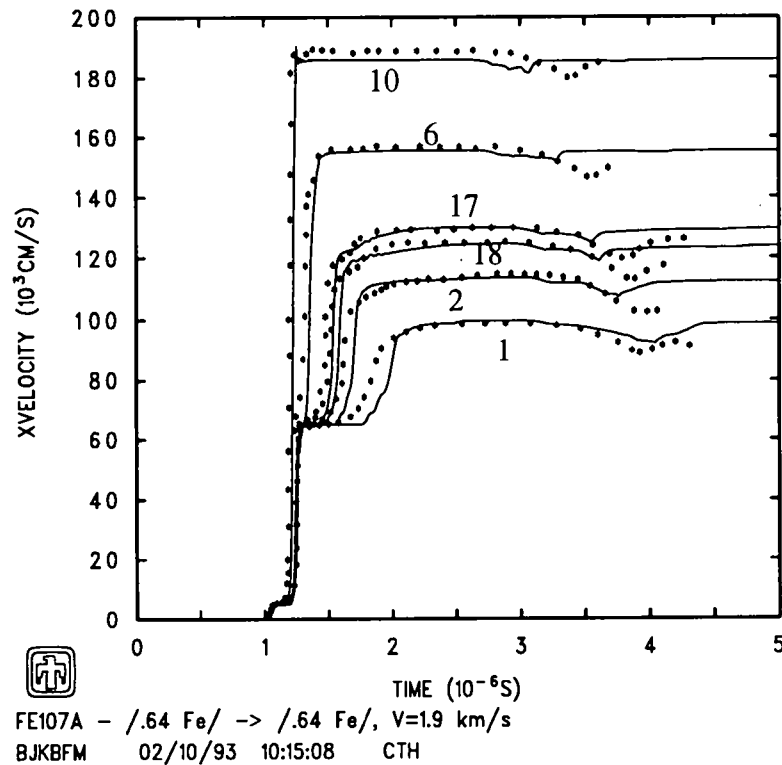


Fig. 10. Calculated free surface velocities for symmetric impacts of 0.64 cm iron plates. Test numbers are given in Ref. [42] and correspond to the following impact velocities: 1 - 0.99, 2 - 1.15, 18 - 1.25, 17 - 1.31, 6 - 1.57, 10 - 1.87 km/s. Discrete points are the experimental data.

Barker and Hollenbach also investigated the unloading behavior of iron in two experiments with a sapphire impactor and a sapphire window, at velocities below the 13 GPa phase transition. Our CTH calculations for their test 15, having an impact velocity of 0.4825 km/s and peak stress of 10.26 GPa, are compared with the measurements (shown by points) in Fig. 11. As noted in the original paper, a calculation using the elastic-perfectly plastic model (shown by the solid line) does not match the unloading behavior. The initial elastic release arrives too early and is too large. For reference, a purely hydrodynamic calculation is also shown (dashed line). The fact that the observed behavior falls in between these two calculations shows that the shocked state retains some strength, but that it is significantly reduced [42].

None of the constitutive models currently used in CTH and other “production” hydrocodes account for this anomalous behavior in iron. The resulting errors in predictions of unloading behavior could have some effect on the comparisons with more complicated experiments, such as those discussed below.

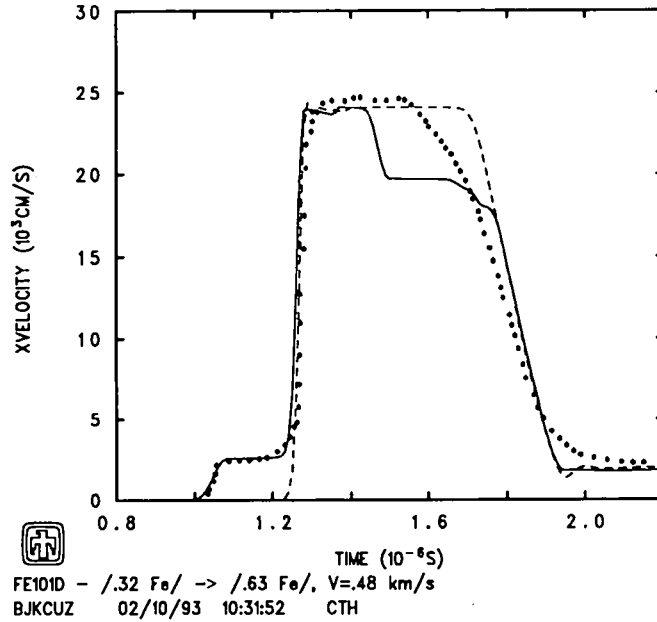


Fig. 11. Calculated velocity at sapphire window for test number 15 of Ref. [42]. The solid line was computed using the elastic-perfectly plastic model, the dashed line using a purely hydrodynamic model. Discrete points are the experimental data.

4.2 Nylon Ball Impact on Iron

Bertholf, et. al. [43] have analyzed an experiment in which a 0.953 cm nylon ball was used to impact a 1.27 cm steel plate with a velocity of 5.182 km/s. Their numerical simulations showed that it was necessary to include the α - ϵ phase transition in the EOS in order to reproduce the observed back-surface spallation of the steel plate.

Our calculations of this experiment, using the CTH code and our new tabular EOS, are shown in Fig. 12. The predictions depend not only on the EOS but are also very sensitive to the treatment of material strength and fracture. In this calculation, we used the Johnson-Cook plasticity model, with parameters for RHA steel [44], and the Johnson-Cook fracture model for steel, with the fracture strength set to 3.8 GPa [43]. The nylon EOS was treated the same as in Ref. [43]. The zone size was 0.032 cm.

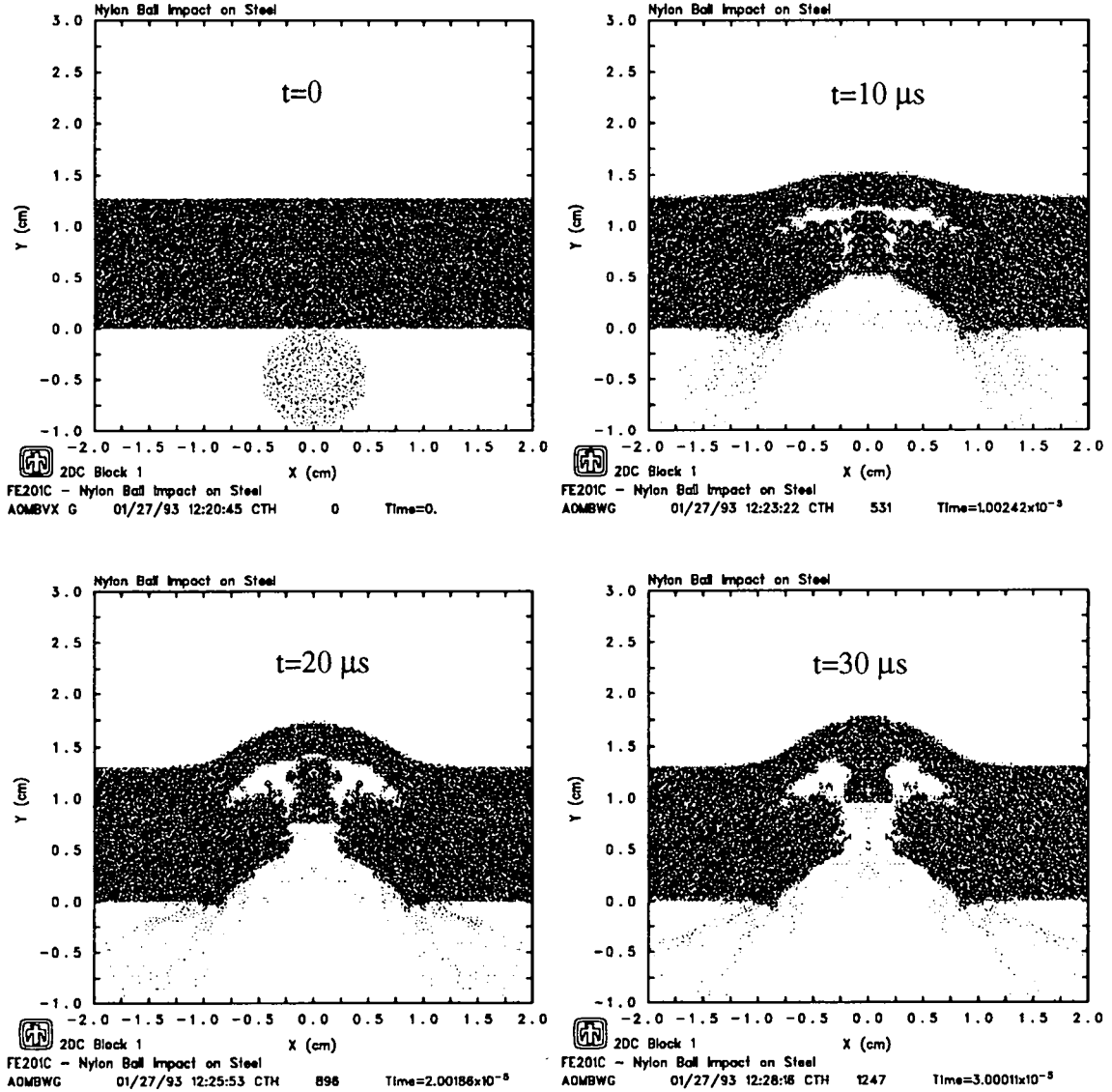


Fig. 12. CTH calculations of nylon ball impacting steel plate.

The principal features of the event, as seen in Fig. 12, are as follows. By 10 μs , the nylon ball has been vaporized and has formed a crater with a depth nearly half the target thickness. Reflection of the impulse from the back surface of the plate has resulted in spallation, opening up a gap. A cylindrical fracture surface has also formed, resulting in a plug of target material. The frames at 20 and 30 μs show the motion of this plug toward the

back surface, opening the gap still further. The existence of the plug and the opening of a wide gap both agree with the experimental data [43].

The dependence of the results on the material parameters is illustrated in Fig. 13. Figure 13a shows a calculation (at 30 μ s) identical to that of Fig. 12, except that the iron EOS table was replaced by a Mie-Grüneisen EOS with no phase transition [45]. There is no evidence of a cylindrical plug, showing that the α - ϵ phase transition is needed to predict that phenomenon. The calculation shown in Fig. 13b (also at 30 μ s) is identical to that of Fig. 12, except that the plasticity parameters for 4340 steel were used instead of those for RHA [44]. Since the strength of 4340 steel is 15% higher than that of RHA, the spall cavity is smaller; the cylindrical plug has formed but has not yet broken loose.

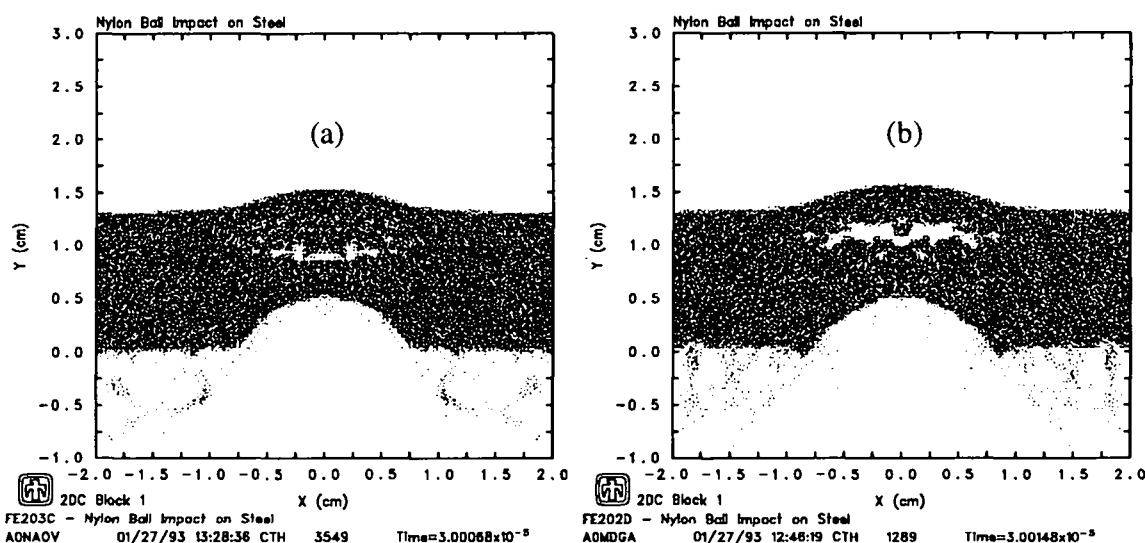


Fig. 13. Sensitivity of nylon-steel impact problem to EOS and material strength: (a) - calculation with Mie-Grüneisen EOS [45], (b) - calculation with 4340 parameters [44]. Both calculations are at 30 μ s.

4.3 Shaped Charge Perforation of RHA Steel

Raftenberg [45] has studied the perforation of a 1.3 cm RHA plate by a shaped charge jet of OFHC copper. He found that the perforation was accomplished by the leading jet particle alone; the velocity (7.73 km/s) and geometry of this particle were determined from radiographs. The splash and debris patterns of the target were recorded on a radiograph taken 36 μ s after impact. The recovered target was sectioned to determine the size and shape of the hole created by the event.

Raftenberg simulated his experiment using a Lagrangian code with an eroding slide line and a simple Mie-Grüneisen EOS with no phase transition. He predicted much too small a

hole using only a tensile failure model, but he was able to obtain reasonable results with a model that included shear band failure effects [45].

Figure 14 shows CTH calculations of this experiment, using our new tabular EOS, the elastic-perfectly plastic model with a yield strength of 1.5 GPa and including thermal softening, and the Johnson-Cook fracture model with a fracture strength of 3.8 GPa. The zone size was 0.0325 cm. The calculations are in very good agreement with the size and shape of the hole observed in the recovered plate (shown by the dark band at 100 μ s). The calculated material distribution at 36 μ s is also consistent with the radiograph (see Ref. [45]).

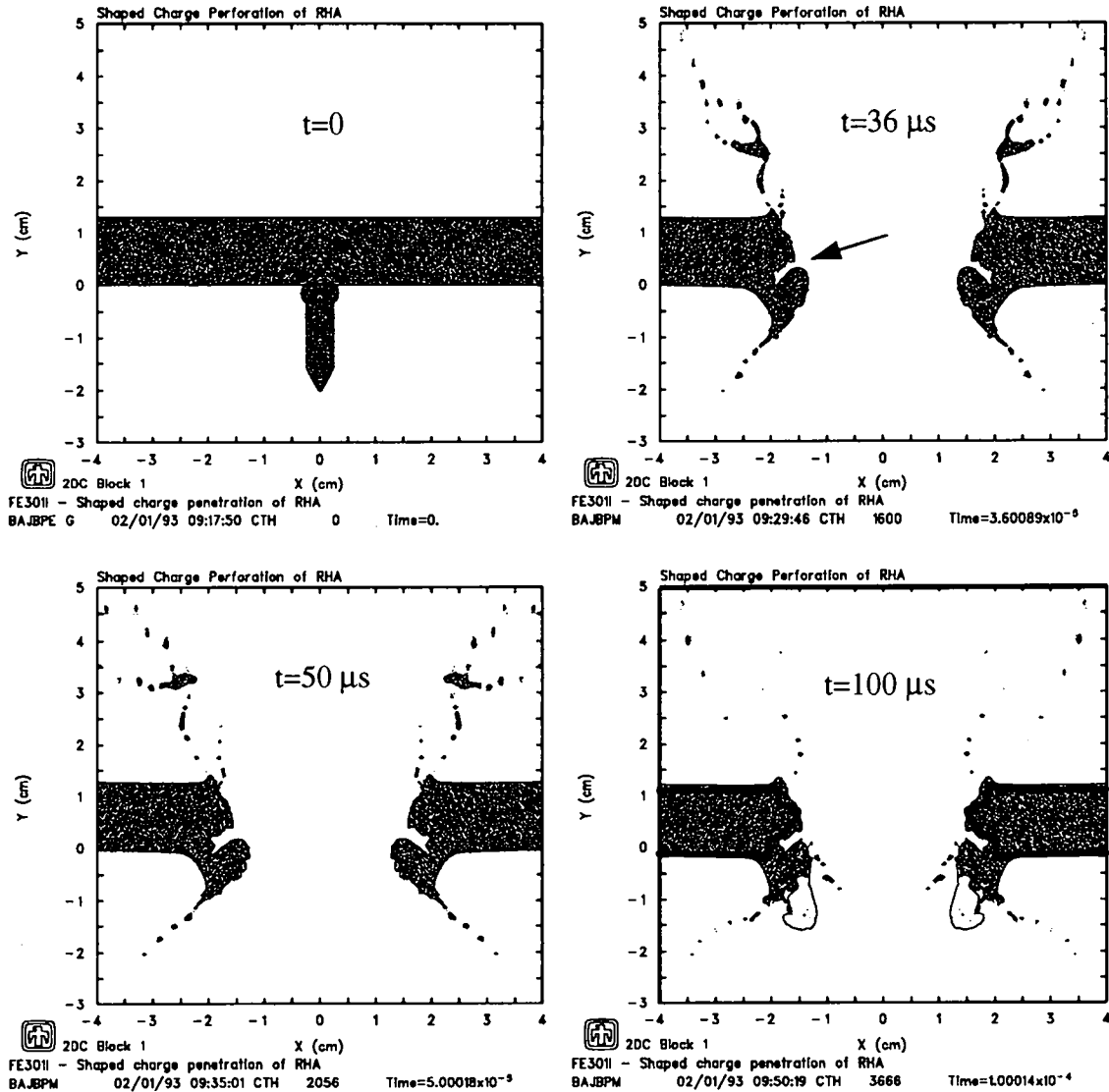


Fig. 14. CTH calculations of perforation of RHA plate by shaped charge jet. The measured hole contours are shown by the dark band on the 100 μ s frame.

An interesting feature of the calculation is the opening of a crack, indicated by an arrow on the 36 μ s frame of Fig. 14, and splitting off of a large piece of material at the hole entrance. (This piece should eventually separate completely from the plate, although the CTH calculations have not predicted it to occur by 100 μ s.) These features are consistent with observations of the recovered plate, including the fact that the entrance hole was larger than the exit hole.

To illustrate the effect of the EOS on the numerical predictions, Fig. 15 shows the results (at 36 μ s) obtained using two other EOS models, but with the same strength and fracture parameters as in Fig. 14. Raftenberg's Mie-Grüneisen EOS [45] with no phase transition was used in Fig. 15a, while the ANEOS model discussed by Bertholf, et. al. [43] was used in Fig. 15b. (The ANEOS model includes the α - ϵ phase transition but ignores melting and other features built into our new EOS; a tabular version, material number 2141 [12], was used in this calculation.) Both calculations show about the same size hole as obtained with our new EOS, but the debris pattern and the behavior near the entrance hole are quite different from those seen in Fig. 14.

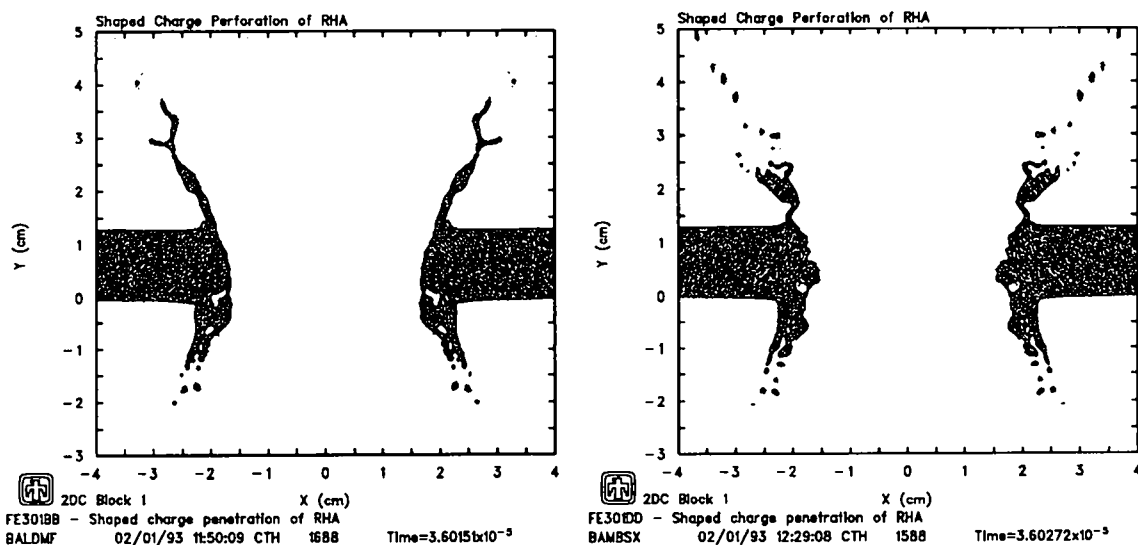


Fig. 15. Sensitivity of RHA perforation problem to EOS: (a) calculation with Mie-Grüneisen EOS [45], (b) - calculation with ANEOS model [12] [43].

However, we must emphasize that the fracture and elastic-plastic models also have a tremendous effect on the predicted results. When the default CTH fracture model is used, the crack discussed above does not appear, although the material distribution at 36 μ s is close to that seen in Fig. 14, otherwise. Surprisingly, the Johnson-Cook plasticity model also gives poor results for this problem. We do not know the reason for this fact, although the levels of stress, strain, temperature, and strain rate encountered in this problem are far outside the regime for which the model was calibrated [44]. Finally, we note that our two-dimensional CTH calculation does not allow fragmentation of the material splitting off from the plate at the entrance hole, an inherently three-dimensional effect.

5. Conclusions

We have developed a new tabular equation of state (EOS) for iron, which includes treatment of solid-solid phase transitions, melting, vaporization, and thermal electronic excitation. The EOS is in good agreement with experimental thermophysical data, static compression data, phase boundaries, and shock-wave measurements. Hydrocode calculations of plate impact tests, the impact of a nylon ball on a steel plate, and the perforation of an RHA steel plate by a shaped charge are also in good agreement with experiment.

In connection with future work, the following points should be considered.

- The model predicts a lower melting temperature at high pressures than has been found in previous analyses. Additional experimental work is required to resolve the differences between existing data and to test the present predictions.
- This EOS does not account for the nonequilibrium and hysteretic behavior of the α - ϵ phase transition. Future extensions of this work could include use of a “two-state” model, with internal state variables, to treat such effects.
- The study of complicated impact experiments shows that the EOS can have a significant effect on hydrocode predictions. However, these predictions are also very dependent on the plasticity and fracture models that are used.
- The study of plate impact experiments shows that existing plasticity models for iron are not satisfactory. In particular, they do not account for the loss of strength in the vicinity of the α - ϵ phase transition and its effect on shock unloading behavior.

Finally, we note that the EOS discussed in this report is applicable only to pure iron and to mildly alloyed steels, such as RHA. It should not be used for stainless steels and other alloys which have significantly different phase boundaries. We have not attempted to construct EOS for such materials, although the present work does lay the foundation for doing that in the future.

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Appendix A

Calculation of Thermal Electronic Entropy Table

The INFERNO calculations reported here were carried out using version 41 of the code, obtained from D. A. Liberman. The entropy was computed at 24 densities, exponentially spaced on the interval $0.6 \leq \rho \leq 600$, and at 28 temperatures, exponentially spaced on the interval $2.3 \times 10^3 \leq T \leq 1.2 \times 10^7$. These results were previously discussed in Refs. [3] and [10].

The Panda IONEQ model [8] computes ionization potentials, energy levels, and statistical weights for atomic ions from a scaling model, using a table of orbital radii and energies for the ground state configuration of the isolated atom [46]. In the present work, the binding energies EA for occupied orbitals were modified to improve agreement between the model predictions and experimental ionization potentials [47]. The old values [46] and modified values (in Hartree) are as follows:

Orbital	EA (old)	EA (mod)
1S+	-2.6394e+02	-2.6394e+02
2S+	-3.2536e+01	-3.0000e+01
2P-	-2.7966e+01	-2.7000e+01
2P+	-2.7441e+01	-2.7000e+01
3S+	-4.3237e+00	-4.1000e+00
3P-	-2.9734e+00	-2.9000e+00
3P+	-2.7538e+00	-2.7000e+00
3D-	-6.3675e-01	-5.0000e-01
3D+	-6.0859e-01	-4.7000e-01
4S+	-2.7116e-01	-2.9765e-01

The IONEQ results were generated using parameter settings $MX=EFAC=3$, $F1=F2=1$, $KS=5$. (The parameter MX is related to the number of allowed configurations, and the parameter KS is used to smooth the entropy table. See the Panda manual [8] for an explanation of the parameters.) The entropy was computed at 50 densities, exponentially spaced on the interval $1.0 \times 10^{-6} \leq \rho \leq 1.0 \times 10^3$, and at 50 temperatures, exponentially spaced on the interval $1.0 \times 10^2 \leq T \leq 1.2 \times 10^8$.

The IONEQ results are quite similar to those from INFERNO; they even agree with the behavior of the entropy isotherms in the insulator-metal transition region. However, the IONEQ model predicts somewhat lower entropies than INFERNO at temperatures in the vicinity of 5.0×10^5 K. We cannot explain the reason for this discrepancy. In any case, the mismatch leads to spurious structure in the pressure when the two data sets were merged to make a composite table. In order to eliminate this problem, the IONEQ entropies were

shifted by subtracting the difference between the IONEQ and INFERNO results at $\rho = 4$ and $1.0 \times 10^5 < T < 1.0 \times 10^6$ at all densities. The transition region was further smoothed by averaging the IONEQ and INFERNO results in the range $1 < \rho < 6$.

Appendix B

Output File for Multiphase EOS Calculation

THE PANDA CODE, UCS VERSION 2.05, 09/09/92
SANDIA NATIONAL LABORATORIES, ALBUQUERQUE, NM 87185

PROBLEM: IRON_EOS DATE: 01/26/93

OPTION?

@doit

!*****

!

! File dated 01/19/93 - Equation of state for alpha-phase iron.
! Tabular cold curve is Birch-Murnaghan fit to static data, with
! R0=7.969, B0=173.0, B0P=4.80. Thermal electronic term is included.
! A tabular term describes the magnetic contribution, which is
! computed from an magnetic specific heat given by:
! for T<= 1042K, CVE = T**1.5/(1080-T)/55.0 cal/mole/K
! for T > 1042K, CVE = 0.
! The energy zero is set to zero density and temperature.

!

!*****

! Setup

sym eb=7.469 seb=-7.469 ro=7.969 bo=173 gam=1.70 deb=425

OPTION?

!

mod sol crv=1 nuc=1 tel=1 tab=1 esft=seb

SOLID-LIQUID MODEL - ENTER MOLECULAR FORMULA

fe

MOLES = 1.0000E+00, Z = 2.6000E+01, AW = 5.5847E+01

FZ = 2.6000E+01, FW = 5.5847E+01, ZAV = 2.6000E+01

ENTER ECOH, RHOREF, TREF, GAMREF, DEBREF, CB, PSSN

7.397 7.873 298 gam deb

COLD CURVE - ENTER ICLD, RTFD, RLJ, FACLJ

4 11 7.0 1

ENTER NAME OF INPUT FILE

tty

ENTER DENSITY AND PRESSURE, POINT BY POINT

6.5000E+00 -2.1681E+01

6.7500E+00 -1.9321E+01

7.0000E+00 -1.6452E+01

7.2500E+00 -1.3046E+01

7.5000E+00 -9.0743E+00

7.7500E+00 -4.5092E+00

8.0000E+00 6.7794E-01

8.2500E+00 6.5157E+00

8.5000E+00 1.3032E+01

8.7500E+00 2.0256E+01

9.0000E+00 2.8215E+01

```

9.2500E+00  3.6939E+01
9.5000E+00  4.6454E+01
9.7500E+00  5.6790E+01
1.0000E+01  6.7975E+01
1.0250E+01  8.0037E+01
1.0500E+01  9.3004E+01
1.0750E+01  1.0690E+02
1.1000E+01  1.2177E+02
1.1250E+01  1.3762E+02
1.1500E+01  1.5449E+02
1.1750E+01  1.7241E+02

```

```

LATTICE VIBRATION MODEL- ENTER INPT, IGRN, RV, TG, GAML
-1 4 - 1 -

```

```

ELECTRONIC TERM - ENTER ENTROPY FILE NAME OR OPTION
elefe

```

```

ENTER MATERIAL NUMBER AND FILE NAME FOR EOS TABLE
100 b100

```

```

OPTION?

```

```

! Make EOS table

```

```

slib sol

```

```

ENTER ID NUMBER FOR TABLE TYPE

```

```

301

```

```

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

```

```

7.0 7.8724 5 1

```

```

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

```

```

7.8724 8.85 11 1

```

```

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

```

```

8.85 13 11 1

```

```

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

```

```

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

```

```

0 298 4 1

```

```

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

```

```

1809 0 1 1

```

```

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

```

```

298 3134 29 2

```

```

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

```

```

800 1200 17 1

```

```

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

```

```

MAKE MAXWELL CONSTRUCTIONS? (YES/NO)

```

```

-

```

```

ENTER ID NUMBER FOR TABLE TYPE

```

```

-

```

```

ENTER MATID, DATE, BINLIB, AND ASCLIB

```

```

101 011993 balp aalp

```

```

OPTION?

```

```

! Make EOS table - high temperature section

```

```

mod sol wsl=1.42

```

```

OPTION?

```

```

slib sol

```

```

ENTER ID NUMBER FOR TABLE TYPE

```

```

301

```

Multiphase Iron EOS

```
MAKE MAXWELL CONSTRUCTIONS? (YES/NO)
-
ENTER ID NUMBER FOR TABLE TYPE
-
ENTER MATID, DATE, BINLIB, AND ASCLIB
101 011893 balpx aalpx
OPTION?
reset
OPTION?
!*****
!
! File dated 01/18/93 - Equation of state for gamma-phase iron.
! Tabular cold curve is Birch-Murnaghan form, with R0=8.060, B0=174.0,
! B0P=4.70. Thermal electronic term is included.
! The energy zero is set to zero density and temperature.
!
!*****
! Setup
sym eb=7.337 seb=-7.337 ro=8.06 bo=174 gam=1.65 deb=300
OPTION?
!
mod sol crv=1 nuc=1 tel=1 esft=seb
SOLID-LIQUID MODEL - ENTER MOLECULAR FORMULA
fe
    MOLES = 1.0000E+00, Z = 2.6000E+01, AW = 5.5847E+01
    FZ = 2.6000E+01, FW = 5.5847E+01, ZAV = 2.6000E+01
ENTER ECOH,RHOREF,TREF,GAMREF,DEBREF,CB,PSSN
7.285 7.9534 298 gam deb
COLD CURVE - ENTER ICLD,RTFD,RLJ,FACLJ
4 11 7.0 1
ENTER NAME OF INPUT FILE
tty
ENTER DENSITY AND PRESSURE, POINT BY POINT
6.5000E+00 -2.2655E+01
6.7500E+00 -2.0390E+01
7.0000E+00 -1.7640E+01
7.2500E+00 -1.4380E+01
7.5000E+00 -1.0583E+01
7.7500E+00 -6.2242E+00
8.0000E+00 -1.2775E+00
8.2500E+00 4.2825E+00
8.5000E+00 1.0481E+01
8.7500E+00 1.7344E+01
9.0000E+00 2.4897E+01
9.2500E+00 3.3164E+01
9.5000E+00 4.2172E+01
9.7500E+00 5.1945E+01
1.0000E+01 6.2509E+01
1.0250E+01 7.3889E+01
1.0500E+01 8.6111E+01
1.0750E+01 9.9199E+01
1.1000E+01 1.1318E+02
1.1250E+01 1.2807E+02
1.1500E+01 1.4391E+02
```

1.1750E+01 1.6072E+02

LATTICE VIBRATION MODEL- ENTER INPT, IGRN, RV, TG, GAML

-1 4 - 1 -

ELECTRONIC TERM - ENTER ENTROPY FILE NAME OR OPTION

elefe

OPTION?

! Make EOS table

slib sol

ENTER ID NUMBER FOR TABLE TYPE

301

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

7.0 7.8724 5 1

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

7.8724 8.85 11 1

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

8.85 13 11 1

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

13 18.5 8 3 298

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

18.5 98 9 3 298

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

1.e3 0 1 1

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

0 298 4 1

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

1809 0 1 1

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

298 3134 29 2

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

3135 6000 9 2

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

6000 2.5e4 12 2

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

2.5e4 1.e5 10 2

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

1.e5 1.2e7 9 2

TEMPERATURE MESH - ENTER TMIN, TMAX, NPTS, MTYPE, RREF

MAKE MAXWELL CONSTRUCTIONS? (YES/NO)

-

ENTER ID NUMBER FOR TABLE TYPE

-

ENTER MATID, DATE, BINLIB, AND ASCLIB

102 011893 bgam agam

OPTION?

reset

OPTION?

!*****

!

! File dated 01/18/93 - Equation of state for epsilon-phase iron.

! Tabular cold curve is Birch-Murnaghan fit to static data, with

Multiphase Iron EOS

```

! R0=8.430, B0=184.0, B0P=5.0. Thermal electronic term is included.
! Energy zero is set to zero density and temperature.
!
!*****
! Setup
sym eb=7.394 seb=-7.394 ro=8.430 bo=182 gam=2.40 deb=385
OPTION?
!
mod sol crv=1 nuc=1 tel=1 esft=seb
SOLID-LIQUID MODEL - ENTER MOLECULAR FORMULA
fe
    MOLES = 1.0000E+00, Z = 2.6000E+01, AW = 5.5847E+01
    FZ = 2.6000E+01, FW = 5.5847E+01, ZAV = 2.6000E+01
ENTER ECOH,RHOREF,TREF,GAMREF,DEBREF,CB,PSSN
7.330 8.264 298 gam deb
COLD CURVE - ENTER ICLD,RTFD,RLJ,FACLJ
4 11 7.5 1
ENTER NAME OF INPUT FILE
tty
ENTER DENSITY AND PRESSURE, POINT BY POINT
7.0000E+00 -2.1536E+01
7.2500E+00 -1.9058E+01
7.5000E+00 -1.6071E+01
7.7500E+00 -1.2546E+01
8.0000E+00 -8.4529E+00
8.2500E+00 -3.7629E+00
8.5000E+00 1.5534E+00
8.7500E+00 7.5251E+00
9.0000E+00 1.4182E+01
9.2500E+00 2.1553E+01
9.5000E+00 2.9667E+01
9.7500E+00 3.8555E+01
1.0000E+01 4.8246E+01
1.0250E+01 5.8769E+01
1.0500E+01 7.0154E+01
1.0750E+01 8.2430E+01
1.1000E+01 9.5628E+01
1.1250E+01 1.0978E+02
1.1500E+01 1.2491E+02
1.1750E+01 1.4105E+02

LATTICE VIBRATION MODEL- ENTER INPT,IGRN,RV,TG,GAML
-1 4 - 2 -
ELECTRONIC TERM - ENTER ENTROPY FILE NAME OR OPTION
elefe
OPTION?
! Make EOS table
slib sol
ENTER ID NUMBER FOR TABLE TYPE
301
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
7.8724 8.85 11 1
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
8.85 13 11 3 298

```



```

DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
13 18.5 8 3 298
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
18.5 98 9 3 298
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
1.e3 0 1 1
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF

TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
0 298 4 1
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
1809 0 1 1
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
298 3134 29 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
3135 6000 9 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
6000 2.5e4 12 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF

MAKE MAXWELL CONSTRUCTIONS? (YES/NO)
-
ENTER ID NUMBER FOR TABLE TYPE
-
ENTER MATID, DATE, BINLIB, AND ASCLIB
103 011893 beps aeps
OPTION?
reset
OPTION?
!*****
!
! File dated 01/18/93 - Equation of state for liquid iron.
! Cold curve parameters are the same as those for the epsilon phase.
! The thermal electronic term is included.
! The energy zero is set to zero density and temperature.
!
!*****
! Setup
sym eb=7.397 seb=-7.397 ro=8.430 bo=182 gam=2.40 deb=385
OPTION?
!
mod sol crv=1 nuc=1 tel=1 esft=seb
SOLID-LIQUID MODEL - ENTER MOLECULAR FORMULA
fe
    MOLES = 1.0000E+00, Z = 2.6000E+01, AW = 5.5847E+01
    FZ = 2.6000E+01, FW = 5.5847E+01, ZAV = 2.6000E+01
ENTER ECOH,RHOREF,TREF,GAMREF,DEBREF,CB,PSSN
7.330 8.264 298 gam deb
COLD CURVE - ENTER ICLD,RTFD,RLJ,FACLJ
4 11 7.5 .68
ENTER NAME OF INPUT FILE
tty
ENTER DENSITY AND PRESSURE, POINT BY POINT
7.0000E+00 -2.1536E+01

```

Multiphase Iron EOS

```

7.2500E+00 -1.9058E+01
7.5000E+00 -1.6071E+01
7.7500E+00 -1.2546E+01
8.0000E+00 -8.4529E+00
8.2500E+00 -3.7629E+00
8.5000E+00 1.5534E+00
8.7500E+00 7.5251E+00
9.0000E+00 1.4182E+01
9.2500E+00 2.1553E+01
9.5000E+00 2.9667E+01
9.7500E+00 3.8555E+01
1.0000E+01 4.8246E+01
1.0250E+01 5.8769E+01
1.0500E+01 7.0154E+01
1.0750E+01 8.2430E+01
1.1000E+01 9.5628E+01
1.1250E+01 1.0978E+02
1.1500E+01 1.2491E+02
1.1750E+01 1.4105E+02

```

LATTICE VIBRATION MODEL- ENTER INPT, IGRN, RV, TG, GAML

1 4 - 2 -

ELECTRONIC TERM - ENTER ENTROPY FILE NAME OR OPTION

elefe

OPTION?

mod liq crs=1 tel=1 esft=seb

CRIS MODEL - ENTER BEXP, EFAC, QFAC, TMIN, NGS, NZI, EPS, DR, DT, XG, WX1, WX2

0 .23 1 - - - - - 2.1 2.1

BFAC, BEXP, EFAC, QFAC = 7.707E+00 7.707E+00 2.300E-01 1.000E+00

TMIN, RFAC, NGS, NZI = 1.023E+03 2.057E-01 1000 1

EPS, DR, DT, XG = 1.000E-05 1.000E-02 1.000E-02 4.000E-01

WX1, WX2 = 2.100E+00 2.100E+00

OPTION?

! Make mesh for EOS table. Note - omit zero density point

! and temperatures below 1000K when making liquid table.

mesh sol

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

1.e-6 1.e-4 7 2

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

1.e-4 2.0 21 2

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

2.0 5.0 16 1

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

5.0 7.8724 12 1

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

7.8724 8.85 11 1

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

8.85 13 11 3 298

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

13 18.5 8 3 298

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

18.5 98 9 3 298

DENSITY MESH - ENTER RMIN, RMAX, NPTS, MTYPE, TREF

1.e3 0 1 1

```

DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF

TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
1809 0 1 1
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
1051.1228 3134 15 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
3135 6000 9 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
6000 2.5e4 12 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
2.5e4 1.e5 10 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
1.e5 1.2e7 9 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF

OPTION?
save mesh msliq
OPTION?
! Make EOS table
slib liq
ENTER ID NUMBER FOR TABLE TYPE
301
MAKE MAXWELL CONSTRUCTIONS? (YES/NO)
no
ENTER ID NUMBER FOR TABLE TYPE
-
ENTER MATID, DATE, BINLIB, AND ASCLIB
104 011893 bliq aliq
OPTION?
reset
OPTION?
!*****
!
! File dated 01/19/93 - Multiphase equation of state for iron.
! The energy zero of the individual tables are set to zero density
! and temperature. The energy zero of the multiphase EOS is set to
! room temperature and zero pressure for the alpha phase.
!
!*****
mod trn
ENTER PHASE SEARCH PARAMETERS - RREF,RCRT,TCRT,PCPS,NCPS,ERR

ENTER MATERIAL NUMBER, FILE NAME, AND ENERGY SHIFT
101 balp 7.3163
ENTER MATERIAL NUMBER, FILE NAME, AND ENERGY SHIFT
101 balpx 7.3924
ENTER MATERIAL NUMBER, FILE NAME, AND ENERGY SHIFT
102 bgam 7.3217 ! shifted by .0054
ENTER MATERIAL NUMBER, FILE NAME, AND ENERGY SHIFT
103 beps 7.3313 ! shifted by .015 (match shock data)
ENTER MATERIAL NUMBER, FILE NAME, AND ENERGY SHIFT
104 bliq 7.3074 ! shifted by -.0089
ENTER MATERIAL NUMBER, FILE NAME, AND ENERGY SHIFT

```

Multiphase Iron EOS

```
5 PHASES SUCCESSFULLY LOADED FOR MODEL
OPTION?
! Make mesh for EOS table
mesh trn
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
0 0 1 1
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
1.e-6 1.e-4 7 2
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
1.e-4 2.0 21 2
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
2.0 5.0 16 1
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
5.0 7.8724 12 1
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
8.409 0 1 1 ! - density at 13.0 GPa transition point
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
7.8724 8.85 10 1
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
8.85 13 11 3 298
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
13 18.5 8 3 298
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
18.5 98 9 3 298
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF
1.e3 0 1 1
DENSITY MESH - ENTER RMIN,RMAX,NPTS,MTYPE,TREF

TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
0 298 4 1
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
1809 0 1 1
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
298 3134 29 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
3135 6000 9 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
6000 2.5e4 12 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
2.5e4 1.e5 10 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF
1.e5 1.2e7 9 2
TEMPERATURE MESH - ENTER TMIN,TMAX,NPTS,MTYPE,RREF

OPTION?
save mesh mstrn
OPTION?
! Make multiphase EOS table
slib trn
ENTER ID NUMBER FOR TABLE TYPE
201
ENTER FZ, FW, PREF, TREF, AND GUESS FOR RHOREF
26.0 55.847 0 298 7.87
```

```

COMPUTED STANDARD STATE - RHOREF, BREF = 7.87238E+00 1.63939E+02
ENTER ID NUMBER FOR TABLE TYPE
301
MAKE MAXWELL CONSTRUCTIONS? (YES/NO)
yes
ENTER TSPALL AND GUESS OF RSPALL
3134 5.15
      T(K)      RV(G/CC)      RL(G/CC)      PV(GPA)      PL(GPA)
ENTER TMIN, TMAX, AND GUESSES FOR RLO AND RUP
3135 2.3e4 2.e-4 5.15
  3.1350E+03  1.7704E-04  5.2024E+00  8.2574E-05  8.3432E-05
  3.4000E+03  4.2890E-04  4.8012E+00  2.1677E-04  2.1788E-04
  3.6874E+03  9.3858E-04  4.5502E+00  5.1364E-04  5.1358E-04
  3.9990E+03  1.8828E-03  4.2946E+00  1.1145E-03  1.1145E-03
  4.3370E+03  3.5066E-03  4.0961E+00  2.2416E-03  2.2413E-03
  4.7036E+03  6.2102E-03  3.9543E+00  4.2783E-03  4.2778E-03
  5.1012E+03  1.0481E-02  3.8390E+00  7.7506E-03  7.7506E-03
  5.5324E+03  1.6957E-02  3.7368E+00  1.3422E-02  1.3421E-02
  6.0000E+03  2.6514E-02  3.6398E+00  2.2347E-02  2.2349E-02
  6.8312E+03  5.2067E-02  3.4685E+00  4.7766E-02  4.7766E-02
  7.7775E+03  9.6267E-02  3.3427E+00  9.4979E-02  9.4979E-02
  8.8549E+03  1.5956E-01  3.2604E+00  1.7620E-01  1.7620E-01
  1.0082E+04  2.4066E-01  3.1708E+00  3.0946E-01  3.0946E-01
  1.1478E+04  3.3520E-01  3.0717E+00  5.1371E-01  5.1371E-01
  1.3068E+04  4.4761E-01  2.9550E+00  8.1560E-01  8.1560E-01
  1.4879E+04  6.0018E-01  2.7870E+00  1.2584E+00  1.2584E+00
  1.6940E+04  7.6153E-01  2.5052E+00  1.8462E+00  1.8462E+00
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